Fermionic Stochastic Schrödinger Equation and Master Equation: An Open System Model

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This paper considers the extension of the non-Markovian stochastic approach for quantum open systems strongly coupled to a fermionic bath, to the models in which the system operators commute with the fermion bath. This technique can also be a useful tool for studying open quantum systems coupled to a spin-chain environment, which can be further transformed into an effective fermionic bath. We derive an exact stochastic Schrödinger equation (SSE), called fermionic quantum state diffusion (QSD) equation, from the first principle by using the fermionic coherent state representation. The reduced density operator for the open system can be recovered from the average of the solutions to the QSD equation over the Grassmann-type noise. By employing the exact fermionic QSD equation, we can derive the corresponding exact master equation. The power of our approach is illustrated by the applications of our stochastic approach to several models of interest including the one-qubit dissipative model, the coupled two-qubit dissipative model, the quantum Brownian motion model and the N-fermion model coupled to a fermionic bath. Different effects caused by the fermionic and bosonic baths on the dynamics of open systems are also discussed.

PACS numbers: 03.65.Yz, 42.50.Lc, 05.40.-a

I. INTRODUCTION

The theory of open quantum systems has experienced a resurgent interest because of the rapid development of quantum experimental technologies and their applications to the fabrication and manipulation of quantum devices (e.g. photonic devices, quantum dots, nanomechanical oscillators). However, an intricate problem exists since in reality no system can be completely isolated from its environment (bath, reservoir etc), and the dynamics of the system of interest will be profoundly affected by the couplings to its environment [1, 2]. When the quantum open systems are coupled to a Markov environment, the Lindblad master equation is a critical tool which can be used to study the dynamics of the open systems [3]. When the Born-Markov approximation is no longer valid, namely, the coupling between system and environment is not weak and the environment cannot be approximated by a broadband bath, one must extend the standard Markov theory to a more general non-Markovian environment. Several attempts to derive the evolution equation of open quantum systems beyond the Markov approximation have been proposed [2, 4–8]. Notably, the non-Markovian quantum state diffusion (QSD) approach developed by Strunz and his coworkers has showed momentous potential of solving large systems (multi-qubit or multi-cavity) [9–15]. Moreover, as a computing tool, many numerical advantages of the QSD approach permit its use in several domains such as high-precision measurement [16], entanglement dynamics [17] and coherence dynamics of the large molecules in biophysics [18] etc. Therefore, it is highly desirable to extend the QSD approach for the bosonic baths to the fermionic case where the non-Markovian features have played increasingly important role [19–23].

The primary theme of our current paper is to establish an exact quantum approach for a class of quantum systems interacting with a fermionic bath. We will consider a class of systems such that the systems and fermionic bath are distinguishable, hence the system Hamiltonian and the bath operators commute. The system of interest in this case may consist of one or more effective particles such as spins, effective fermions etc. The case where the system and bath operators ant-commute will be covered in-depth in a separate paper [24]. It is noted that the commutative model we proposed arises from many physical settings including spin bath and fermionic bath (e.g. see Appendix A).

We will derive a fermionic stochastic Schrödinger equation for an open quantum system embedded in a fermionic bath, called the fermionic QSD equation. To illustrate the power of our approach, we solve several models as examples by using this new technique, including a one-qubit dissipative model, a two-qubit dissipative model, the quantum Brownian motion in a fermionic bath and a multiple-particle model. In the first example, we give the explicit analytical solution without any approximation in a special case. In the second example, we show how to construct the crucial $\hat{Q}$ operator contained in the fermionic QSD equation. In the third example, we consider a continuous variable model where a Brownian particle is immersed in a bath of fermion particles.

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The last example involves a genuine multi-particle system that has been solved exactly by our QSD approach. Finally, the difference between the bosonic bath and the fermonic bath is discussed.

This paper is organized as follows. In section II, we introduce the general commutative fermionic bath model and derive the fundamental dynamic equation for this model. In section III, we derive the formal exact master equation from the QSD equation. In section IV, we present a simple example of using this fermionic QSD approach to solve the one-qubit dissipative model. In section V, we solve the two-qubit dissipative model to show the construction of some complicated $\hat{Q}$ operator. In section VI, we apply our fermionic QSD approach to a continuous variable model to solve the quantum Brownian motion model in a fermionic bath. In section VII, we solve a genuine multi-partite system, the N-fermion model, to show that our approach is not only applicable to small systems (one-qubit or two-qubit), but is also applicable to large quantum open systems. Based on the last example, we also evaluate the differences between the bosonic bath and the fermonic bath. Finally, in section VIII, we conclude the paper. In Appendix A, we provide an effective commutative model consisting of spinless fermions as an environment. In Appendix B and C, we present the details of derivation of the non-Markovian QSD equation for a fermionic bath. In Appendix D, we prove a Novikov-type theorem for a Grassmann Gaussian stochastic process, which plays a crucial role in deriving the exact master equation from the corresponding stochastic Schrödinger equation. In Appendix E-F, we derive explicit equations of motion for the coefficients of the master equation for the examples presented in this paper.

II. NON-MARKOVIAN QSD EQUATION FOR AN OPEN SYSTEM COUPLED TO A FERMIONIC BATH

For a quantum open system interacting with a fermionic environment, the total Hamiltonian may be written as

$$\hat{H}_{\text{tot}} = \hat{H}_{\text{s}} + \hat{H}_{\text{b}} + \hat{H}_{\text{int}}, \tag{1}$$

where $\hat{H}_{\text{s}}$ is the Hamiltonian of the system, $\hat{H}_{\text{b}}$ is the Hamiltonian of the bath and $\hat{H}_{\text{int}}$ is the interaction term. When we consider the fermionic bath, $\hat{H}_{\text{b}}$ and $\hat{H}_{\text{int}}$ can be written as (setting $\hbar = 1$ throughout the paper)

$$\hat{H}_{\text{b}} = \sum_i \omega_i \hat{c}_i^\dagger \hat{c}_i, \tag{2}$$

$$\hat{H}_{\text{int}} = \sum_i (g_i^* \hat{c}_i^\dagger \hat{L} + g_i \hat{L}^\dagger \hat{c}_i), \tag{3}$$

where $\hat{c}_i^\dagger$ and $\hat{c}_i$ are fermionic creation and annihilation operators $\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}$. Here we emphasize that the bath may consist of a set fermions or spins (e.g. see [26]; An example is shown in Appendix A.)

In the interaction picture, the total Hamiltonian becomes

$$\hat{H}_{\text{tot}}(t) = \hat{H}_{\text{s}} + \sum_i (g_i^* e^{i\omega_i t} \hat{c}_i^\dagger \hat{L} + g_i e^{-i\omega_i t} \hat{L}^\dagger \hat{c}_i). \tag{4}$$

We use the fermionic coherent state (e.g., see [27, 28]) to describe the state of environment. For a single mode, the fermionic coherent state is defined as

$$\hat{c}_i |\xi_i\rangle = \xi_i |\xi_i\rangle, \tag{5}$$

where ξ_i is a Grassmann variable which satisfies the following properties $\{\xi_i, \xi_j\} = 0$, $\{\xi_i, \xi_j^*\} = 0$. Generally, the coherent state can be expanded in terms of Fock states as $|\xi_i\rangle = |0\rangle - \xi_i c_i^\dagger |0\rangle$. The coherent states (ket and bra vectors) for the multi-mode environment are given by $|\xi\rangle = |\xi_1\rangle \otimes |\xi_2\rangle \otimes |\xi_3\rangle \otimes ...$ and $\langle\xi| = \langle\xi_1| \otimes \langle\xi_2| \otimes \langle\xi_3| \otimes ....$

Now, we can define

$$\psi_t(\xi^*) = \langle\xi|\psi_{\text{tot}}(t)\rangle, \tag{6}$$

where $|\psi_{\text{tot}}(t)\rangle$ is the total state vector for the system and environment, and $\langle\xi|$ is a coherent state representation for the environment. In this paper, we focus on the case where the initial state of the bath is vacuum state. The finite temperature bath will be discussed in [24] by using the Bogoliubov transformation [29]. With the coherent state representation, we can derive the non-Markovian QSD equation for the fermionic bath as

$$\frac{\partial}{\partial t}\psi_t(\xi^*) = [-i\hat{H}_{\text{s}} + \hat{L}\xi_t^* - \hat{L}^\dagger \int_0^t ds K(t,s) \frac{\delta_l}{\delta \xi_s^*}]\psi_t(\xi^*), \tag{7}$$

where $\xi_t^* = -i\sum_i g_i^* e^{i\omega_i t} \xi_i^*$ and $K(t,s) = \sum_i |g_i|^2 e^{-i\omega_i (t-s)}$ is the correlation function. (Details of the derivation can be found in Appendix B) We use $\frac{\delta_l}{\delta\xi_s^*}\psi_t(\xi^*)$ to denote the left-functional-derivative with respect to the Grassmann variables. Our fermionic approach is applicable to arbitrary correlation functions especially for the general non-Markovian case.

Similar to the formal bosonic QSD equation [9], the fermionic QSD contains a time-nonlocal Grassmann functional derivative which renders a direct application of the derived fermionic QSD extremely difficult, if not impossible. In order to find a time-local QSD equation, one can introduce a time-dependent operator (also ξ^*-dependent in general) $\hat{Q}$, defined as

$$\frac{\delta_l \psi_t(\xi^*)}{\delta \xi_s^*} = \hat{Q}(t,s,\xi^*)\psi_t(\xi^*). \tag{8}$$

If no confusion arise, we will use the shorthand notation: $\hat{Q} = \hat{Q}(t,s,\xi^*)$. With this $\hat{Q}$ operator, the exact stochastic QSD equation can be written as

$$\frac{\partial}{\partial t}\psi_t(\xi^*) = [-i\hat{H}_{\text{s}} + \hat{L}\xi_t^* - \hat{L}^\dagger \bar{Q}]\psi_t(\xi^*), \tag{9}$$

where $\bar{Q}(t,\xi^*) = \int_0^t ds K(t,s)\hat{Q}(t,s,\xi^*)$. The stochastic QSD equation for a fermionic bath we have presented here is an exact equation of motion for the open quantum system directly derived from the microscopic Hamiltonian without any approximation. It should be noted that in our derivation of the QSD equation, we have not explicitly specified the system Hamiltonian and the coupling operators, $\hat{H}_{\rm s}$ and $\hat{L}$. Here we have introduced a new type of stochastic process ξ_t^*. The solution of our QSD equation is called a Grassmann quantum trajectory. By construction, the reduced density matrix of the open system can be recovered by the statistical mean over the Grassmann noise. Although the fermionic QSD equation looks formally similar to the bosonic case, the dynamic behaviors of the system governed by the two types of equations can be different due to distinct differences between the bosonic and fermionic particles. Mathematically, the most striking difference between the bosonic and fermionic QSD equations is that the former contains a complex Gaussian noise while the latter is driven by a non-commutative Grassmann Gausian noise.We will illustrate the difference in a concrete example in a subsequent section.

In order to derive the dynamic equation for the $\hat{Q}$ operator, we consider the consistency condition (CC),

$$\frac{\delta_l}{\delta\xi_s^*}\frac{\partial}{\partial t}\psi_t(\xi^*) = \frac{\partial}{\partial t}\frac{\delta_l}{\delta\xi_s^*}\psi_t(\xi^*). \tag{10}$$

Applying the QSD Eq. (9) to CC, the equation for $\hat{Q}$ operator is derived as

$$\begin{aligned}\frac{\partial}{\partial t}\hat{Q} &= -i[\hat{H}_{\rm s},\hat{Q}] - \{\hat{L}\xi_t^*,\hat{Q}\} \\ &\quad - \hat{L}^\dagger\bar{Q}(-\xi^*)\hat{Q} + \hat{Q}\hat{L}^\dagger\bar{Q} - \hat{L}^\dagger\frac{\delta}{\delta\xi_s^*}\bar{Q},\end{aligned} \tag{11}$$

where the sign of $\bar{Q}(-\xi^*)$ depends on the functional form of noise contained in $\bar{Q}$. (Details of derivation and discussion can be found in Appendix C.) The initial condition for the $\hat{Q}$ operator is

$$\hat{Q}(t,s=t,\xi^*) = \hat{L}. \tag{12}$$

However, for a simple case that $\hat{Q}$ is independent of Grassmann noise, the equation for the $\hat{Q}$ reduces to

$$\frac{\partial}{\partial t}\hat{Q} = -i[\hat{H}_{\rm s},\hat{Q}] - \{\hat{L}\xi_t^*,\hat{Q}\} - [\hat{L}^\dagger\bar{Q},\hat{Q}]. \tag{13}$$

Eq. (11) and Eq. (13) can be used to determine the exact $\hat{Q}$ operator. However, for most practical problems, it may be a daunting task to determine the exact $\hat{Q}$. Therefore, it is important to develop a perturbation approach similar to that developed for the bosonic bath [10]. In fact, we may expand $\hat{Q}$ operator as

$$\begin{aligned}\hat{Q}(t,s,\xi^*) &= \hat{Q}^{(0)}(t,s) + \int_0^t \hat{Q}^{(1)}(t,s,s_1)\xi_{s_1}^* ds_1 \\ &\quad + \int_0^t\int_0^t \hat{Q}^{(2)}(t,s,s_1,s_2)\xi_{s_1}^*\xi_{s_2}^* ds_1 ds_2 + ... \\ &\quad + \int_0^t ... \int_0^t \hat{Q}^{(n)}(t,s,s_1,...s_n)\xi_{s_1}^*...\xi_{s_n}^* ds_1...ds_n \\ &\quad + ...\end{aligned} \tag{14}$$

Substituting this equation into Eq. (11), one can derive the dynamic equations of the coefficients for each order $\hat{Q}^{(i)}$. Particularly, the zeroth-order term $\hat{Q}^{(0)}(t,s)$ will satisfy the following equation (neglect all the noise terms)

$$\frac{\partial}{\partial t}\hat{Q}^{(0)}(t,s) = -i[\hat{H}_{\rm s},\hat{Q}^{(0)}(t,s)] - [\hat{L}^\dagger\bar{Q}^{(0)}(t),\hat{Q}^{(0)}(t,s)], \tag{15}$$

where $\bar{Q}^{(0)}(t) = \int_0^t \hat{Q}^{(0)}(t,s)K(t,s)ds$, and the initial condition is

$$\hat{Q}^{(0)}(t,s=t) = \hat{L}. \tag{16}$$

III. FORMAL EXACT MASTER EQUATION FOR AN OPEN QUANTUM SYSTEM COUPLED TO A FERMIONIC BATH

Now, we will derive the master equation governing the reduced density operator of the open quantum system from the stochastic QSD equation (9). First, we define the stochastic density operator as

$$\hat{P}_t = |\psi_t(\xi^*)\rangle\,\langle\psi_t(-\xi)| \tag{17}$$

It is easy to verify that the reduced density matrix of the open system can be written as

$$\begin{aligned}\hat{\rho} &= \sum_n \langle n|\psi_{\rm tot}\rangle\langle\psi_{\rm tot}|n\rangle \\ &= \int\prod\nolimits_i d\xi_i^* d\xi_i e^{-\sum_j \xi_j^*\xi_j}\sum_n \langle n|\xi\rangle\langle\xi|\psi_{\rm tot}\rangle\langle\psi_{\rm tot}|n\rangle \\ &= \int\prod\nolimits_i d\xi_i^* d\xi_i e^{-\sum_j \xi_j^*\xi_j}\sum_n \langle\xi|\psi_{\rm tot}\rangle\langle\psi_{\rm tot}|n\rangle\langle n|-\xi\rangle \\ &= \int\prod\nolimits_i d\xi_i^* d\xi_i e^{-\sum_j \xi_j^*\xi_j}\hat{P}_t \\ &= \langle\hat{P}_t\rangle_s\end{aligned} \tag{18}$$

where $\langle ...\rangle_s$ denotes the statistical mean over the Grassmann Gaussian noise defined by

$$\langle ...\rangle_s \equiv \int\prod\nolimits_i d\xi_i^* d\xi_i e^{-\sum_j \xi_j^*\xi_j}(...). \tag{19}$$

From this expression, we say that the reduced density matrix can be unraveled by a set of Grassmann quantum trajectories $|\psi_t(\xi^*)\rangle$.

From the QSD equation Eq. (9), we have

$$\frac{\partial}{\partial t}\langle\psi_t(-\xi)| = \langle\psi_t(-\xi)|\,[i\hat{H}_{\rm s} - \xi_t\hat{L}^\dagger - \bar{Q}^\dagger(t,-\xi)\hat{L}], \quad (20)$$

thus,

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho} &= \frac{\partial}{\partial t}\langle\hat{P}_t\rangle_s \\ &= \langle(-i\hat{H}_{\rm s} + \hat{L}\xi_t^* - \hat{L}^\dagger\bar{Q})\hat{P}_t\rangle_s \\ &+ \langle\hat{P}_t(i\hat{H}_{\rm s} - \xi_t\hat{L}^\dagger - \bar{Q}^\dagger(-\xi)\hat{L})\rangle_s \\ &= -i[\hat{H}_{\rm s},\hat{\rho}] + \hat{L}\langle\xi_t^*\hat{P}_t\rangle_s - \langle\hat{P}_t\xi_t\rangle_s\hat{L}^\dagger \\ &- \hat{L}^\dagger\langle\bar{Q}\hat{P}_t\rangle_s - \langle\hat{P}_t\bar{Q}^\dagger(-\xi)\rangle_s\hat{L}. \quad (21)\end{aligned}$$

In order to establish the exact master equation from the fermionic QSD equation (9), one needs to handle the terms $\langle\hat{P}_t\xi_t\rangle_s$ etc. In fact, we can prove a Novikov-type theorem for the Grassmann Gaussian noise (see Appendix D),

$$\langle\hat{P}_t\xi_t\rangle_s = -\langle\bar{Q}\hat{P}_t\rangle_s, \quad (22)$$
$$\langle\xi_t^*\hat{P}_t\rangle_s = \langle\hat{P}_t\bar{Q}^\dagger(-\xi)\rangle_s. \quad (23)$$

With the help of the Novikov-type theorem for the Grassmann noise, the exact master equation can be written as

$$\frac{\partial}{\partial t}\hat{\rho} = -i[\hat{H}_{\rm s},\hat{\rho}] + [\hat{L},\langle\hat{P}_t\bar{Q}^\dagger(-\xi)\rangle_s] + [\langle\bar{Q}\hat{P}_t\rangle_s,\hat{L}^\dagger]. \quad (24)$$

If the operator $\hat{Q}$ is independent of the Grassmann noise, then the exact master equation is immediately obtained,

$$\frac{\partial}{\partial t}\hat{\rho} = -i[\hat{H}_{\rm s},\hat{\rho}] + [\hat{L},\hat{\rho}\bar{Q}^\dagger] + [\bar{Q}\hat{\rho},\hat{L}^\dagger]. \quad (25)$$

Moreover, in the Markov limit, $\bar{Q} = \gamma_f\hat{L}$, this master equation reduces to the standard Lindblad master equation:

$$\frac{\partial}{\partial t}\hat{\rho} = -i[\hat{H}_{\rm s},\hat{\rho}] + \gamma_f[\hat{L},\hat{\rho}\hat{L}^\dagger] + \gamma_f[\hat{L}\hat{\rho},\hat{L}^\dagger]. \quad (26)$$

In subsequent sections, we will derive several interesting master equations from the corresponding QSD equations.

IV. EXAMPLE 1: ONE-QUBIT DISSIPATIVE MODEL

We start with a very simple example, one-qubit in fermionic bath. This is a special case where it is possible to derive the fully analytical solution without any approximation.

A. Master equation and non-Markovian quantum dynamics

The total Hamiltonian for the one-qubit dissipative model may be written as

$$\hat{H}_{\rm tot} = \hat{H}_{\rm s} + \hat{H}_{\rm b} + \hat{H}_{\rm int}, \quad (27)$$

$$\hat{H}_{\rm s} = \frac{\omega}{2}\hat{\sigma}_z, \quad (28)$$

$$\hat{H}_{\rm b} = \sum_i \omega_i\hat{c}_i^\dagger\hat{c}_i, \quad (29)$$

$$\hat{H}_{\rm int} = \sum_i (g_i^*\hat{c}_i^\dagger\hat{L} + g_i\hat{L}^\dagger\hat{c}_i), \quad (30)$$

where $\hat{L} = \hat{\sigma}_-$ for this particular model.

From Eq. (13), the solution for the $\hat{Q}$ can be obtained as

$$\hat{Q}(t,s) = x_1(t,s)\hat{\sigma}_-, \quad (31)$$

with the initial condition

$$\hat{Q}(t,s=t) = \hat{L} = \hat{\sigma}_-, \quad (32)$$

and the coefficient $x_1(t,s)$ is shown to satisfy

$$\frac{\partial}{\partial t}x_1(t,s) = [i\omega + X_1(t)]x_1(t,s), \quad (33)$$

where $X_1(t) = \int_0^t x_1(t,s)K(t,s)ds$, and $K(t,s)$ is the correlation function, and the initial condition is given by $x_1(t,s) = 1$.

Thus, the exact $\hat{Q}$ operator can be fully determined. It is worth noting that this $\hat{Q}$ operator has the same form as the bosonic case [10]. Finally, the explicit QSD equation for this model is

$$\frac{\partial}{\partial t}\psi_t(\xi^*) = [-i\frac{\omega}{2}\hat{\sigma}_z + \hat{\sigma}_-\xi_t^* - X_1(t)\hat{\sigma}_+\hat{\sigma}_-]\psi_t(\xi^*), \quad (34)$$

and the exact master equation is

$$\begin{aligned}\frac{d}{dt}\hat{\rho} &= -i[\hat{H}_{\rm s},\hat{\rho}] + [\hat{L},\hat{\rho}\hat{Q}^\dagger] + [\hat{Q}\hat{\rho},\hat{L}^\dagger] \\ &= -i\frac{\omega}{2}(\hat{\sigma}_z\hat{\rho} - \hat{\rho}\hat{\sigma}_z) + X_1^*(t)(\hat{\sigma}_-\hat{\rho}\hat{\sigma}_+ - \hat{\rho}\hat{\sigma}_+\hat{\sigma}_-) \\ &+ X_1(t)(\hat{\sigma}_-\hat{\rho}\hat{\sigma}_+ - \hat{\sigma}_+\hat{\sigma}_-\hat{\rho}). \quad (35)\end{aligned}$$

With this exact master equation, the dynamics of this model can be fully determined.

B. A limiting case – the environment consists of only one fermion

Now, we consider a very special case for the one-qubit model where the "environment" [30] contains only one fermion. By analytically solving this model, we show explicitly that the fermionic QSD gives rise to identical results to those predicted by the ordinary quantum mechanics. The model is described by the following Hamiltonian,

$$\hat{H}_{\rm tot} = \frac{\omega}{2}\hat{\sigma}_z + \omega_b\hat{c}^\dagger\hat{c} + (g^*\hat{\sigma}_-\hat{c}^\dagger + g\hat{\sigma}_+\hat{c}), \quad (36)$$

and the zero-temperature correlation function becomes

$$K(t,s) = |g|^2 e^{-i\omega_b(t-s)}. \tag{37}$$

Substituting the correlation function into the expression of $X_1(t) = \int_0^t x_1(t,s)K(t,s)ds$, we will find the differential equation for $X_1(t)$ as

$$\frac{\partial}{\partial t}X_1(t) = |g|^2 - i\omega_b X_1(t) + i\omega X_1(t) + X_1(t)^2. \tag{38}$$

For simplicity, we consider the resonance case, then the solution $X_1(t)$ can reduce to

$$X_1(t) = |g|\tan(|g|\,t). \tag{39}$$

From the master equation Eq. (35), we can calculate time evolution for the off-diagonal elements in the density matrix.

$$\frac{d}{dt}\hat{\rho}_{21} = \frac{d}{dt}\langle\hat{\sigma}_+\rangle = Tr(\frac{d}{dt}\hat{\rho}\hat{\sigma}_+) = i\omega\hat{\rho}_{21} - X_1^*(t)\hat{\rho}_{21}. \tag{40}$$

Finally, we can derive the time evolution for $\hat{\rho}_{21}$ as

$$\hat{\rho}_{21}(t) = \hat{\rho}_{21}(0)e^{i\omega t}\cos\left[|g|\,t\right]. \tag{41}$$

Similarly, we can get

$$\hat{\rho}_{12}(t) = \hat{\rho}_{12}(0)e^{-i\omega t}\cos\left[|g|\,t\right]. \tag{42}$$

This result shows that the coherence (off-diagonal elements in density matrix) will decrease and increase periodically.

On the other hand, we can easily solve this simple case using elementary quantum mechanics. Since this is only a two-body problem, we can solve the evolution for the whole system in a straightforward manner. One can check that elementary quantum mechanics gives rise to the identical results obtained by the fermionic QSD approach in Eq. (41,42).

V. EXAMPLE 2: COUPLED TWO-QUBIT DISSIPATIVE MODEL

In this section, we consider a system containing a pair of coupled two-level systems (spins or some other effective two-level models) interacting with a common fermionic bath. We will show how to construct exact and approximate $\hat{Q}$ operator in this example. The total Hamiltonian of this model can be written as,

$$\hat{H}_{\rm tot} = \hat{H}_{\rm s} + \hat{H}_{\rm b} + \hat{H}_{\rm int}, \tag{43}$$

where

$$\begin{aligned}
\hat{H}_{\rm s} &= \omega_A\hat{\sigma}_z^A + \omega_B\hat{\sigma}_z^B + J_{xy}(\hat{\sigma}_+^A\hat{\sigma}_-^B + \hat{\sigma}_-^A\hat{\sigma}_+^B) + J_z\hat{\sigma}_z^A\hat{\sigma}_z^B, \\
\hat{H}_{\rm b} &= \sum_j \omega_j\hat{c}_j^\dagger\hat{c}_j, \\
\hat{H}_{\rm int} &= \sum_j (g_j\hat{c}_j^\dagger\hat{L} + g_j^*\hat{c}_j\hat{L}^\dagger),
\end{aligned} \tag{44}$$

Here, the operator $\hat{L} = \kappa_A\hat{\sigma}_-^A + \kappa_B\hat{\sigma}_-^B$ describles the pattern of interaction to the environment. κ_A and κ_B are constants describing different coupling strengths for the two qubits.

The perturbative zeroth-order $\hat{Q}$ operator can be derived as

$$\hat{Q}^{(0)}(t,s) = \sum_{i=1}^{4} f_i(t,s)\hat{Q}_i \tag{45}$$

where $\hat{Q}_i$ $(i = 1,2,3,4)$ are the time-independent basis operators, and $f_i(t,s)$ are time-dependent coefficients.

The four basis operators in terms of the Pauli matrices may be written as

$$\hat{Q}_1 = \hat{\sigma}_-^A,\ \hat{Q}_2 = \hat{\sigma}_-^B,\ \hat{Q}_3 = \hat{\sigma}_z^A\hat{\sigma}_-^B,\ \ \hat{Q}_4 = \hat{\sigma}_z^B\hat{\sigma}_-^A, \tag{46}$$

From Eq. (15), we can derive the differential equation for the coefficients as

$$\frac{\partial}{\partial t}f_1(t,s) = +2i\omega_A f_1 - iJ_{xy}f_3 + 2iJ_z f_4 + \kappa_A F_1 f_1 - \kappa_B F_1 f_3 + \kappa_B F_3 f_1 + \kappa_B F_3 f_4 + \kappa_B F_4 f_3 + \kappa_A F_4 f_4, \tag{47}$$

$$\frac{\partial}{\partial t}f_2(t,s) = +2i\omega_B f_2 - iJ_{xy}f_4 + 2iJ_z f_3 + \kappa_B F_2 f_2 - \kappa_A F_2 f_4 + \kappa_B F_3 f_3 + \kappa_A F_3 f_4 + \kappa_A F_4 f_2 + \kappa_A F_4 f_3, \tag{48}$$

$$\frac{\partial}{\partial t}f_3(t,s) = +2i\omega_B f_3 - iJ_{xy}f_1 + 2iJ_z f_2 - \kappa_A F_2 f_1 + \kappa_B F_2 f_3 + \kappa_A F_3 f_1 + \kappa_A F_4 f_2 + \kappa_B F_3 f_2 + \kappa_A F_4 f_3, \tag{49}$$

$$\frac{\partial}{\partial t}f_4(t,s) = +2i\omega_A f_4 - iJ_{xy}f_2 + 2iJ_z f_1 - \kappa_B F_1 f_2 + \kappa_A F_1 f_4 + \kappa_B F_3 f_1 + \kappa_B F_3 f_4 + \kappa_A F_4 f_1 + \kappa_B F_4 f_2, \tag{50}$$

where $F_i(t) = \int_0^t ds K(t,s) f_i(t,s)$ $(i = 1, 2, 3, 4)$, and the initial conditions are

$$f_1(t, s = t) = \kappa_A, \quad (51)$$
$$f_2(t, s = t) = \kappa_B, \quad (52)$$
$$f_3(t, s = t) = 0, \quad (53)$$
$$f_4(t, s = t) = 0, \quad (54)$$

Moreover, we can also determine the exact $\hat{Q}$ operator for this two-qubit model. We can verify rigorously that the exact $\hat{Q}$ operator contains five terms where the last term is noise-dependent. The details of the derivation is presented in Appendix E. If we use this zeroth-order $\hat{Q}$ operator, the master equation can be explicitly written in the following form

$$\frac{d}{dt}\hat{\rho} = -i[\hat{H}_{\rm s}\hat{\rho} - \hat{\rho}\hat{H}_{\rm s}] + \{\sum_{i=1}^{4} F_i^*[\hat{L}\hat{\rho}\bar{Q}_i^\dagger - \hat{\rho}\bar{Q}_i^\dagger\hat{L}] + H.C.\}. \quad (55)$$

Next, we consider a simple case, in which all the parameters are symmetric for two qubits, i.e. $\omega_A = \omega_B = \omega$, $\kappa_A = \kappa_B = 1$. Then, we can derive the following master equation

$$\begin{aligned}\frac{d}{dt}\hat{\rho} &= -i[\hat{H}_{\rm s}, \hat{\rho}] + [\hat{L}, \hat{\rho}\bar{Q}^\dagger] + [\bar{Q}\hat{\rho}, \hat{L}^\dagger] \\ &= -i\omega[(\hat{\sigma}_z^A + \hat{\sigma}_z^B)\hat{\rho} - \hat{\rho}(\hat{\sigma}_z^A + \hat{\sigma}_z^B)] \\ &- iJ_{xy}[(\hat{\sigma}_+^A\hat{\sigma}_-^B + \hat{\sigma}_+^B\hat{\sigma}_-^A)\hat{\rho} - \hat{\rho}(\hat{\sigma}_+^A\hat{\sigma}_-^B + \hat{\sigma}_+^B\hat{\sigma}_-^A)] \\ &- iJ_z[\hat{\sigma}_z^A\hat{\sigma}_z^B\hat{\rho} - \hat{\rho}\hat{\sigma}_z^A\hat{\sigma}_z^B] \\ &+ \{F_1^*[(\hat{\sigma}_-^A + \hat{\sigma}_-^B)\hat{\rho}\hat{\sigma}_+^A - \hat{\rho}\hat{\sigma}_+^A(\hat{\sigma}_-^A + \hat{\sigma}_-^B)] \\ &+ F_2^*[(\hat{\sigma}_-^A + \hat{\sigma}_-^B)\hat{\rho}\hat{\sigma}_+^B - \hat{\rho}\hat{\sigma}_+^B(\hat{\sigma}_-^A + \hat{\sigma}_-^B)] \\ &+ F_3^*[(\hat{\sigma}_-^A + \hat{\sigma}_-^B)\hat{\rho}\hat{\sigma}_z^A\hat{\sigma}_+^B - \hat{\rho}\hat{\sigma}_z^A\hat{\sigma}_+^B(\hat{\sigma}_-^A + \hat{\sigma}_-^B)] \\ &+ F_4^*[(\hat{\sigma}_-^A + \hat{\sigma}_-^B)\hat{\rho}\hat{\sigma}_z^B\hat{\sigma}_+^A - \hat{\rho}\hat{\sigma}_z^B\hat{\sigma}_+^A(\hat{\sigma}_-^A + \hat{\sigma}_-^B)] + H.C.\}.\end{aligned} \quad (56)$$

The master equation derived above is valid for a general correlation function. For numerical simulations, one need to consider a special example of the correlation function. A general correlation function may be written as

$$K(t,s) = \int_0^\infty d\omega J(\omega)[\coth(\omega/2k_BT)\cos\omega(t-s) - i\sin\omega(t-s)], \quad (57)$$

where $J(\omega)$ is the spectral density. If we choose $J(\omega) = \Gamma\omega e^{-(\frac{\omega}{\omega_c})}$, which is so-called Ohmic case, the correlation function in the zero-temperature can be written as

$$K(t,s) = \frac{\Gamma}{[\frac{1}{\omega_c} + i(t-s)]^2}, \quad (58)$$

where ω_c is the cut-off frequency.

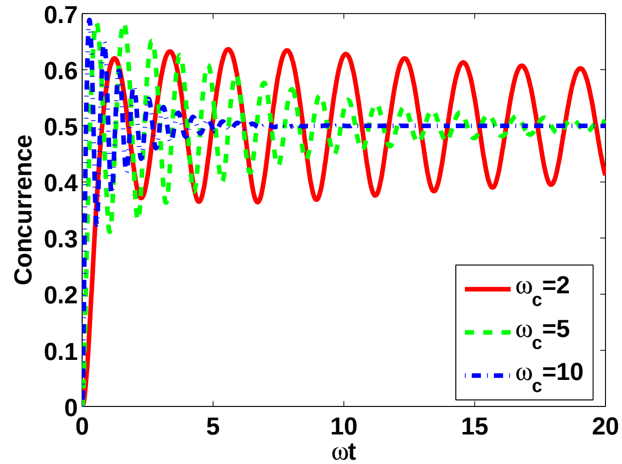

FIG. 1: Time evolution of concurrence for different ω_c.

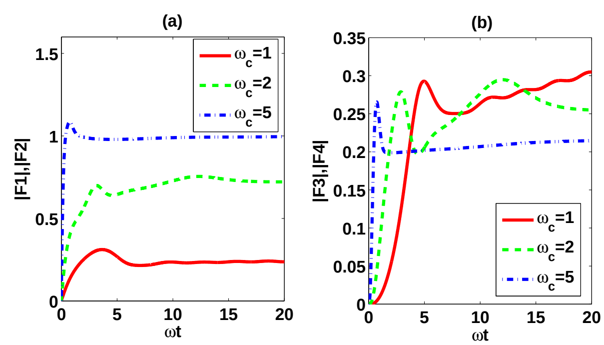

FIG. 2: Time evolution of $|F_1(t)|$, $|F_2(t)|$, $|F_3(t)|$, and $|F_4(t)|$. In the symmetric case, $|F_1(t)| = |F_2(t)|$, $|F_3(t)| = |F_4(t)|$. The parameters are $\omega_1 = \omega_2 = \omega = 1$,

VI. EXAMPLE 3: QUANTUM BROWNIAN PARTICLE IN A FERMIONIC BATH

We consider a continuous model consisting of a Brownian particle interacting with a fermionic bath. The Hamiltonian of the Brownian particle is given by,

$$\hat{H}_{\rm s} = \omega_m(\hat{p}^2 + \hat{q}^2). \quad (59)$$

The Hamiltonian of the fermionic bath is

$$\hat{H}_{\rm b} = \sum_i \omega_i \hat{c}_i^\dagger \hat{c}_i, \quad (60)$$

and the interaction Hamiltonian is given by

$$\hat{H}_{\rm int} = \hat{q}\sum_i(g_i^*\hat{c}_i^\dagger + g_i\hat{c}_i). \quad (61)$$

So, the total Hamiltonian is

$$\hat{H}_{\text{tot}} = \hat{H}_{\text{s}} + \hat{H}_{\text{b}} + \hat{H}_{\text{int}}. \tag{62}$$

Applying our QSD approach to this model, it can be easily shown that $\hat{Q}$ operator takes the following form:

$$\begin{aligned}\hat{Q} &= x_1(t,s)\hat{q} + x_2(t,s)\hat{p} + x_3(t,s,\xi^*)\hat{p}\hat{q} \\ &+ x_4(t,s,\xi^*)\hat{p}^2 + x_5(t,s,\xi^*)\hat{q}^2 + ... \end{aligned}\tag{63}$$

which is a infinite series, therefore, it is difficult to determine the exact $\hat{Q}$ operator. A useful approximation is to neglect all the noise-dependent terms, after which we obtain the so-called zeroth-order approximate $\hat{Q}$ as

$$\hat{Q} \approx x_1(t,s)\hat{q} + x_2(t,s)\hat{p}. \tag{64}$$

Substituting this approximate $\hat{Q}$ operator into Eq. (15), we can derive the differential equations for the coefficients $x_1(t,s)$ and $x_2(t,s)$ as

$$\frac{\partial}{\partial t}x_1(t,s) = 2\omega_m x_2(t,s) + iX_2(t)x_1(t,s) - 2iX_1(t)x_2(t,s), \tag{65}$$

$$\frac{\partial}{\partial t}x_2(t,s) = -2\omega_m x_1(t,s) - iX_2(t)x_2(t,s). \tag{66}$$

The initial conditions for coefficients $x_1(t,s)$ and $x_2(t,s)$ are

$$x_1(t,s=t) = 1, \tag{67}$$

$$x_2(t,s=t) = 0. \tag{68}$$

Using this approximate $\hat{Q}$ operator, the master equation can be written as

$$\begin{aligned}\frac{d}{dt}\hat{\rho} &= -i[\hat{H}_{\text{s}},\hat{\rho}] + [\hat{L},\hat{\rho}\bar{Q}^\dagger] + [\bar{Q}\hat{\rho},\hat{L}^\dagger] \\ &= -i\omega_m[(\hat{p}^2+\hat{q}^2)\hat{\rho} - \hat{\rho}(\hat{p}^2+\hat{q}^2)] \\ &+ \{X_1^*[\hat{q}\hat{\rho}\hat{q} - \hat{\rho}\hat{q}\hat{q}] + X_2^*[\hat{q}\hat{\rho}\hat{p} - \hat{\rho}\hat{p}\hat{q}] + H.C.\}. \end{aligned}\tag{69}$$

It should be noted that the X_2^* (including its conjugation X_2) does not exist in the Markov limit. Hence, the approximate $\hat{Q}$ operator defined above is different from the Markov approximation. It is also different from the weak-coupling approximation since the approximate $\hat{Q}$ still contains the higher-order terms of the coupling constant. We expect that the master equation obtained from the approximate $\hat{Q}$ will be valid in a weakly non-Markovian regime.

From the master equation we can derive the evolution equations for all the mean values of operators $\hat{q},\hat{p}$,

$$\frac{d}{dt}\langle\hat{q}\rangle = 2\omega_m\langle\hat{p}\rangle, \tag{70}$$

$$\frac{d}{dt}\langle\hat{p}\rangle = -2\omega_m\langle\hat{q}\rangle - iX_1^*\langle\hat{q}\rangle - iX_2^*\langle\hat{p}\rangle + iX_1\langle\hat{q}\rangle + iX_2\langle\hat{p}\rangle. \tag{71}$$

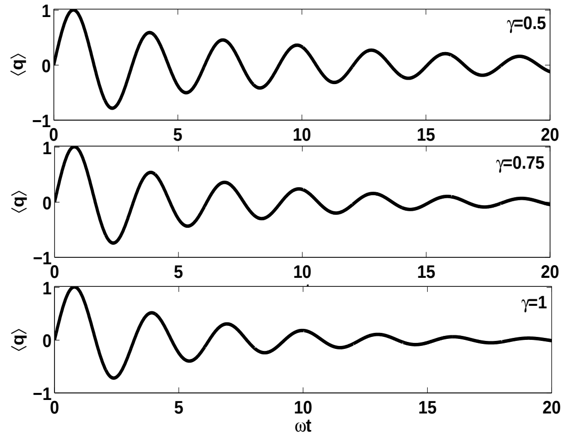

FIG. 3: Time evolution of mean values of operator $\hat{q}$ in different environments. The parameter γ indicates the memory effect. The other parameters are $\omega_m = \omega = 1$, $\Omega = \pi/2$.

In Fig. 3, we plot the time evolution of $\langle\hat{q}\rangle$ in different kinds of environments with different γ. In order to show the transition from non-Markovian to Markovian, Ornstein-Uhlenbeck noise $K(t,s) = \frac{\gamma}{2}e^{-(\gamma+i\Omega)|t-s|}$ is chosen in our numerical simulations. The reason of using Ornstein-Uhlenbeck noise is that the memory time of the environment can be described by one parameter $1/\gamma$. Fig. 3 shows how the evolution of $\langle\hat{q}\rangle$ is affected by γ. This is a unique phenomenon in the non-Markovian case.

VII. EXAMPLE 4. N-FERMION SYSTEM COUPLED TO A FERMIONIC BATH

A. Dynamic equation for the general N-fermion model

In the last example, we will establish the exact time-local fermionic QSD equation and master equation for a genuine multipartite system coupled to a fermionic bath. We show that, using the fermionic QSD approach, the exact $\hat{Q}$ operator of the N-qubit model can be easily determined.

More specifically, let us consider the following Hamiltonian

$$\hat{H}_{\text{tot}} = \hat{H}_{\text{s}} + \hat{H}_{\text{b}} + \hat{H}_{\text{int}}, \tag{72}$$

$$\hat{H}_{\text{b}} = \sum_{j=1}^{N_b}\omega_j\hat{c}_j^\dagger\hat{c}_j, \tag{73}$$

$$\hat{H}_{\text{int}} = \sum_{j=1}^{N_b}g_j(\hat{c}_j^\dagger\hat{L} + \hat{L}^\dagger\hat{c}_j). \tag{74}$$

where $\hat{H}_{\text{b}}$ is a fermionic bath. We assume that the system

of interest consists of N fermions, i.e.

$$\hat{H}_{\rm s} = \sum_{i=1}^{N_s} A_i \hat{a}_i^\dagger \hat{a}_i, \tag{75}$$

here, $\hat{a}_i^\dagger$ and $\hat{a}_i$ are also fermion creation and annihilation operators; the Lindblad operator is

$$\hat{L} = \sum_{i=1}^{N_s} \hat{a}_i. \tag{76}$$

This Hamiltonian could be an effective Hamiltonian transformed from a set of spins. For example, suppose that we have a long chain with N sites, if the first $N_s (N_s < N)$ sites are treated as system and the other N_b sites are treated as bath ($N_s + N_b = N$), then performing the Jordan-Wigner transformations for both the system and the bath, we may result in this type of effective Hamiltonian (for details, see Appendix A).

We can show that the exact $\hat{Q}$ operator of this model takes the following form

$$\hat{Q} = \sum_{i=1}^{N_s} x_i(t,s)\hat{a}_i, \tag{77}$$

and the differential equation for the coefficients in $\hat{Q}$ operator are given by

$$\frac{\partial}{\partial t} x_j(t,s) = iA_j x_j(t,s) + \sum_i^{N_s} X_j(t) x_i(t,s), \tag{78}$$

where $X_j(t) = \int_0^t K(t,s) x_j(t,s) ds$. So, $\bar{Q}(t) = \sum_{i=1}^{N_s} X_i(t)\hat{a}_i$. The exact master equation of this model is

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho} &= -i[\hat{H}_{\rm s}, \hat{\rho}] + [\hat{L}, \hat{\rho}\bar{Q}^\dagger] + [\bar{Q}\hat{\rho}, \hat{L}^\dagger] \\ &= -i[\hat{H}_{\rm s}, \hat{\rho}] + [\sum_{i=1}^{N_s} \hat{a}_i, \hat{\rho} \sum_i^{N_s} X_i^*(t)\hat{a}^\dagger] \\ &\quad + [(\sum_{i=1}^{N_s} X_i(t)\hat{a}_i)\hat{\rho}, \sum_{i=1}^{N_s} \hat{a}_i^\dagger]. \end{aligned} \tag{79}$$

B. Fermionic versus bosonic baths

It is instructive to consider a simple case with two fermions in the system ($N_s = 2$). The Hamiltonian is then given by

$$\hat{H}_{\rm s} = \omega_1 \hat{a}_1^\dagger \hat{a}_1 + \omega_2 \hat{a}_2^\dagger \hat{a}_2, \tag{80}$$

$$\hat{L} = \hat{a}_1 + \hat{a}_2, \tag{81}$$

it is easy to show that the exact $\bar{Q}$ operator is

$$\bar{Q} = X_1(t)\hat{a}_1 + X_2(t)\hat{a}_2 \tag{82}$$

where $X_1(t,s)$ and $X_2(t,s)$ can be determined in Eq. (78) as $N_s = 2$ case. Then, the explicit master equation can be written as

$$\begin{aligned}\frac{d}{dt}\hat{\rho} &= -i\omega_1(\hat{a}_1^\dagger\hat{a}_1\hat{\rho} - \hat{\rho}\hat{a}_1^\dagger\hat{a}_1) - i\omega_2(\hat{a}_2^\dagger\hat{a}_2\hat{\rho} - \hat{\rho}\hat{a}_2^\dagger\hat{a}_2) \\ &\quad + \{X_1^*(t)(\hat{a}_1\hat{\rho}\hat{a}_1^\dagger - \hat{\rho}\hat{a}_1^\dagger\hat{a}_1) + X_1^*(t)(\hat{a}_2\hat{\rho}\hat{a}_1^\dagger - \hat{\rho}\hat{a}_1^\dagger\hat{a}_2) \\ &\quad + X_2^*(t)(\hat{a}_1\hat{\rho}\hat{a}_2^\dagger - \hat{\rho}\hat{a}_2^\dagger\hat{a}_1) + X_2^*(t)(\hat{a}_2\hat{\rho}\hat{a}_2^\dagger - \hat{\rho}\hat{a}_2^\dagger\hat{a}_2) \\ &\quad + H.C.\}. \end{aligned} \tag{83}$$

On the other hand, we can also solve this model exactly if the two effective fermions (spins) are coupled to a bosonic bath. The Hamiltonian takes the same form as Eq. (72-76), except that $\hat{c}_j$ ($\hat{c}_j^\dagger$) represent bosonic annihilation (creation) operators (also consider $N_s = 2$ case). Using the non-Markovian QSD approach for bosonic bath [9], the bosonic QSD equation can be derived as

$$\frac{\partial}{\partial t}\psi_t(z^*) = [-i\hat{H}_{\rm s} + \hat{L}z_t^* - \hat{L}^\dagger\bar{O}]\psi_t(z^*), \tag{84}$$

where $\bar{O}(t,z^*) = \int_0^t ds K(t,s)\hat{O}(t,s,z^*)$. In the bosonic QSD equation, the noise $z_t^* = -i\sum_i g_i^* e^{i\omega_i t} z_i^*$ is the complex (not Grassmann) Gaussian noise. The exact $\bar{O}$ operator is determined as follows

$$\begin{aligned}\bar{O}(t,z^*) &= X_1(t)\hat{a}_1 + X_2(t)\hat{a}_2 + X_3(t)\hat{a}_1^\dagger\hat{a}_1\hat{a}_2 \\ &\quad + X_4(t)\hat{a}_2^\dagger\hat{a}_1\hat{a}_2 + i\int_0^t ds' X_5(t,s') z_{s'}^* \hat{a}_1\hat{a}_2. \end{aligned} \tag{85}$$

Details about the coefficients can be found in Appendix F.

We use this particular example to illustrate different aspects between the fermionic and bosonic baths. As shown above, we can find the exact $\hat{Q}$ ($\hat{O}$) operators for both the fermnionic bath and the bosonic counterpart. Since the exact dynamic evolution of the system will be fully determined by $\hat{Q}$ ($\hat{O}$) operators, so we may compare the difference between the two operators given in Eq. (82) and Eq. (85), respectively. The first two terms $X_1(t,s)$ and $X_2(t,s)$ are the same for both the $\hat{Q}$ and $\hat{O}$ operators (one can easily check that they satisfy the same equations), and the difference comes from other terms. In the cases where $X_1(t,s)$ and $X_2(t,s)$ are dominant, one would not expects sharp difference between the fermionic and bosonic baths. For example, when $\omega_1 = \omega_2$, two operators $\hat{Q}$ and $\hat{O}$ are exactly the same. However, we found that the extra terms $X_3(t,s)$ and $X_4(t,s)$ occurred in $\hat{O}$ may become important under certain conditions as shown in Fig. 4 where the coefficients in the $\hat{O}$ and $\hat{Q}$ operators are plotted. Clearly, the fermionic and bosonic baths may result in very different dynamics. In the numerical simulations, we choose the Ornstein-Uhlenbeck noise $K(t,s) = \frac{\gamma}{2} e^{-(\gamma + i\Omega)|t-s|}$ for simplicity. However, our approach is applicable for arbitrary kinds of correlation function.

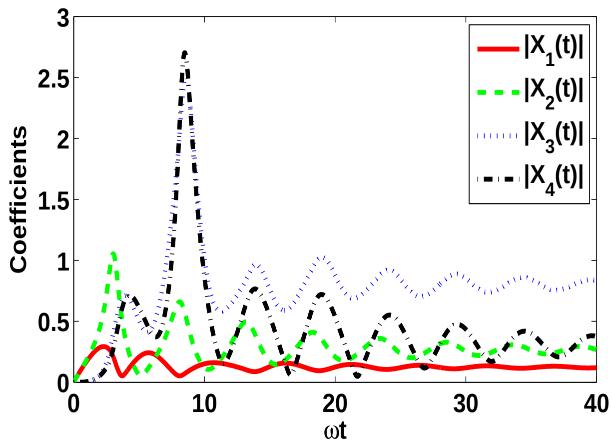

FIG. 4: Dynamic evolution of the coefficients in $\bar{Q}$ (for fermionic bath) and $\bar{O}$ (for bosonic bath) operators. The parameters are $\omega_1 = 2$, $\omega_2 = \omega = 1$, $\gamma = 0.4$, $\Omega = \pi/4$.

VIII. CONCLUSION

In summarizing, we have developed a novel technique called the fermionic quantum state diffusion approach which is a useful tool for studying quantum open systems coupled to a fermionic bath. Using the Grassmann coherent state, the exact fermionic QSD equation and the corresponding master equation are derived for several physically interesting models. We have shown that the time-local QSD approach developed in this paper can efficiently solve open systems coupled to fermionic baths by employing the exact or approximate $\hat{Q}$ operators. Moreover, our research also suggests that some spin bath problems can also be solved by using the effective fermion bath. Finally, it is of great interest to apply the fermionic QSD approach to more realistic models such as finite temperature fermion baths and large spin baths, and we leave these topics open for future discussion.

Acknowledgements

We thank Prof. J. H. Eberly, Prof. N. J. M. Horing, Prof. B. L. Hu, and Dr. J. Jing for useful discussions and the support by grants from the NSF PHY-0925174, AFOSR No. FA9550-12-1-0001, Ikerbasque Foundation Startup, the Basque Government (grant IT472-10) and the Spanish MEC (Project No. FIS2009-12773-C02-02).

Appendix A: Spin chain as an effective fermion bath model

In this section, we consider a spin-chain model where some spins are treated as the system of interest, the rest is treated as its environment. We show that the model can be transformed to a fermionic bath model.

Consider a quantum system interacting with a XX spin chain. The Hamiltonian is

$$\hat{H}_{\rm tot} = \hat{H}_{\rm s} + \hat{H}_{\rm b} + \hat{H}_{\rm int}, \tag{A1}$$

$$\hat{H}_{\rm b} = \sum_i (\hat{\sigma}_i^+ \hat{\sigma}_{i+1}^- + \hat{\sigma}_{i+1}^+ \hat{\sigma}_i^-), \tag{A2}$$

$$\hat{H}_{\rm int} = \hat{L}^\dagger \hat{\sigma}_1 + \hat{\sigma}_1^\dagger \hat{L}. \tag{A3}$$

After performing the Jordan-Wigner transformation,

$$\hat{\sigma}_j^- = \exp(-i\pi \sum_{k=1}^{j-1} \hat{c}_k^\dagger \hat{c}_k) \hat{c}_j, \tag{A4}$$

and the Fourier transformation [26],

$$\hat{c}_j = \frac{1}{\sqrt{N}} \sum_{p=-N/2}^{N/2} \exp(-ij\phi_p) \hat{a}_p, \tag{A5}$$

the original Hamiltonian Eq. (A1-A3) become

$$\hat{H}_{\rm tot} = \hat{H}_{\rm s} + \hat{H}_{\rm b} + \hat{H}_{\rm int}, \tag{A6}$$

$$\hat{H}_{\rm b} = \sum_{p=-N/2}^{N/2} 2\cos\phi_p \hat{a}_p^\dagger \hat{a}_p, \tag{A7}$$

$$\hat{H}_{\rm int} = \frac{1}{\sqrt{N}} \sum_{p=-N/2}^{N/2} [\hat{L}^\dagger \exp(-i\phi_p) \hat{a}_p + \exp(i\phi_p) \hat{a}_p^\dagger \hat{L}]. \tag{A8}$$

This effective Hamiltonian obtained from the transformation takes the same form given by Eq. (1-3). Therefore, we may use the QSD approach to study the dynamics of the subsystem of the spin-chain model.

Appendix B: Derivation of the non-Markovian QSD equation for a fermionic bath

To start with, we list several useful commutation relations between fermionic coherent state and operators:

$$\begin{aligned} &\langle \xi_i | \hat{L} = \hat{L} \langle \xi_i |, \ \langle \xi_i | \hat{H}_{\rm s} = \hat{H}_{\rm s} \langle \xi_i |, \\ &\langle \xi_i | \hat{c}_i = \frac{\partial_l}{\partial \xi_i^*} \langle \xi_i |, \ \langle \xi_i | \hat{c}_i^\dagger = \langle \xi_i | \xi_i^* = \xi_i^* \langle \xi_i |. \end{aligned} \tag{B1}$$

Using these relations, we can derive the QSD equation as

$$\begin{aligned} &\frac{\partial}{\partial t} \psi_t(\xi^*) \\ &= -i \langle \xi | \hat{H}_{\rm tot}(t) | \psi_{\rm tot}(t) \rangle \\ &= -i \langle \xi | \hat{H}_{\rm s} + \sum_i (g_i^* e^{i\omega_i t} \hat{c}_i^\dagger \hat{L} + H.C.) | \psi_{\rm tot}(t) \rangle \\ &= -i \hat{H}_{\rm s} \psi_t(\xi^*) + \hat{L} \xi_t^* \psi_t(\xi^*) \\ &- i \hat{L}^\dagger \sum_i g_i e^{-i\omega_i t} \langle \xi | \hat{c}_i | \psi_{\rm tot}(t) \rangle, \end{aligned} \tag{B2}$$

where $\xi_t^* = -i\sum_i g_i^* e^{i\omega_i t}\xi_i^*$. Then using the chain rule to introduce the functional derivative,

$$\langle \xi|\hat{c}_i|\psi_{\rm tot}(t)\rangle = \frac{\partial_l}{\partial \xi_i^*}\psi_t(\xi^*) \tag{B3}$$

$$= \int ds \frac{\partial \xi_s^*}{\partial \xi_i^*}\frac{\delta_l}{\delta \xi_s^*}\psi_t(\xi^*). \tag{B4}$$

Finally, we have

$$\frac{\partial}{\partial t}\psi_t(\xi^*) = [-i\hat{H}_{\rm s} + \hat{L}\xi_t^* - \hat{L}^\dagger \int ds K(t,s)\frac{\delta_l}{\delta \xi_s^*}]\psi_t(\xi^*), \tag{B5}$$

where $K(t,s) = \sum_i |g_i|^2 e^{-i\omega_i(t-s)}$. This is just the final QSD equation.

Appendix C: Equation for $\hat{Q}$ operator

First, consider the following two commutation relations:

$$\frac{\delta_l}{\delta \xi_s^*}[\xi_t^*\psi_t(\xi^*)] = -\xi_t^*\frac{\delta_l}{\delta \xi_s^*}\psi_t(\xi^*) \tag{C1}$$

and

$$\frac{\delta_l}{\delta \xi_s^*}[\bar{Q}\psi_t(\xi^*)] = \bar{Q}(-\xi^*)\hat{Q}\psi_t(\xi^*) + (\frac{\delta_l}{\delta \xi_s^*}\bar{Q})\psi_t(\xi^*), \tag{C2}$$

for fixed order of $\hat{Q}$ operator. One can prove them easily.

With Eq. (C1) and Eq. (C2), we can apply the consistency condition to $\psi_t(\xi^*)$.

$$\frac{\delta_l}{\delta \xi_s^*}\frac{\partial}{\partial t}\psi_t(\xi^*) = \frac{\partial}{\partial t}\frac{\delta_l}{\delta \xi_s^*}\psi_t(\xi^*). \tag{C3}$$

The left-hand side is

$$\begin{aligned} LHS =& [-i\hat{H}_{\rm s}\hat{Q} - \hat{L}\xi_t^*\hat{Q} \\ & - \hat{L}^\dagger(\frac{\delta}{\delta \xi_s^*}\bar{Q}) - \hat{L}^\dagger\bar{Q}(-\xi^*)\hat{Q}]\psi_t(\xi^*). \end{aligned} \tag{C4}$$

On the other hand, the right-hand side becomes

$$RHS = \frac{\partial}{\partial t}(\hat{Q})\psi_t(\xi^*) + [-i\hat{Q}\hat{H}_{\rm s} + \hat{Q}\hat{L}\xi_t^* - \hat{Q}\hat{L}^\dagger\bar{Q}]\psi_t(\xi^*). \tag{C5}$$

Equate LHS and RHS and eliminate $\psi_t(\xi^*)$, we have

$$\begin{aligned} \frac{\partial}{\partial t}\hat{Q} =& -i[\hat{H}_{\rm s},\hat{Q}] - \{\hat{L}\xi_t^*,\hat{Q}\} \\ & - \hat{L}^\dagger\bar{Q}(-\xi^*)\hat{Q} + \hat{Q}\hat{L}^\dagger\bar{Q} - \hat{L}^\dagger\frac{\delta_l}{\delta \xi_s^*}\bar{Q}. \end{aligned} \tag{C6}$$

Appendix D: Proof of Novikov-type theorem for the Grassmann noise

In this section, we will provide a proof of Novikov-type theorem for a Grassmann Gaussian noise, which plays a crucial role in deriving the exact or approximate master equations from the corresponding stochastic Schrödinger equations.

Theorem: Suppose that ξ_t, ξ_t^* are Grassmann-type Gaussian processes and the $\hat{P}_t$ is the stochastic density operator, then we have the following two identities:

$$\langle \hat{P}_t\xi_t\rangle_s = -\langle \bar{Q}(\xi^*)\hat{P}_t\rangle_s, \tag{D1}$$

$$\langle \xi_t^*\hat{P}_t\rangle_s = \langle \hat{P}_t\bar{Q}^\dagger(-\xi)\rangle_s. \tag{D2}$$

Proof:

$$\begin{aligned} & \langle \hat{P}_t\xi_t\rangle_s \\ =& \int \prod_i d\xi_i^* d\xi_i e^{-\sum_i \xi_i^*\xi_i} |\psi(\xi^*)\rangle \langle \psi(-\xi)| (i\sum_j g_j e^{-i\omega_j t}\xi_j) \\ =& -i\sum_j g_j e^{-i\omega_j t}\int \prod_i d\xi_i^* d\xi_i [|\psi(\xi^*)\rangle\langle\psi(-\xi)| \frac{\partial_l}{\partial \xi_j^*}(e^{-\sum_i \xi_i^*\xi_i})] \\ =& i\sum_j g_j e^{-i\omega_j t}\int \prod_i d\xi_i^* d\xi_i (\frac{\partial_l}{\partial(-\xi_j^*)}|\psi(\xi^*)\rangle\langle\psi(-\xi)|)e^{-\sum_i \xi_i^*\xi_i} \\ =& -i\sum_j g_j e^{-i\omega_j t}\int \prod_i d\xi_i^* d\xi_i [e^{-\sum_i \xi_i^*\xi_i}(\int ds \frac{\partial \xi_s^*}{\partial \xi_j^*}\frac{\delta_l}{\delta \xi_s^*})\hat{P}_t] \\ =& -\int ds \sum_j |g_j|^2 e^{-i\omega_j(t-s)}\int \prod_i d\xi_i^* d\xi_i [e^{-\sum_i \xi_i^*\xi_i}\frac{\delta_l}{\delta \xi_s^*}\hat{P}_t] \\ =& -\int \prod_i d\xi_i^* d\xi_i e^{-\sum_i \xi_i^*\xi_i}\int ds K(t,s)\hat{Q}(t,s,\xi^*)\hat{P}_t] \\ =& -\langle \bar{Q}\hat{P}_t\rangle_s. \end{aligned} \tag{D3}$$

Similarly, we can prove

$$\langle \xi_t^* \hat{P}_t \rangle_s = \langle \hat{P}_t \bar{Q}^\dagger(-\xi) \rangle_s. \tag{D4}$$

This concludes our proof of the Novikov-type theorem for the Grassmann Gaussian noise.

Appendix E: Exact $\hat{Q}$ operator for the two-qubit model

For the coupled two-qubit model, the exact $\hat{Q}$ takes the following form:

$$\begin{aligned}\hat{Q}(t,s,\xi^*) &= f_1(t,s)\hat{Q}_1 + f_2(t,s)\hat{Q}_2 + f_3(t,s)\hat{Q}_3 \\ &+ f_4(t,s)\hat{Q}_4 + i\int_0^t ds' f_5(t,s,s')\xi_{s'}^* \hat{Q}_5,\end{aligned} \tag{E1}$$

where the basis operators are given by

$$\begin{aligned}&\hat{Q}_1 = \hat{\sigma}_-^A,\ \hat{Q}_2 = \hat{\sigma}_-^B,\ \hat{Q}_3 = \hat{\sigma}_z^A \hat{\sigma}_-^B, \\ &\hat{Q}_4 = \hat{\sigma}_z^B \hat{\sigma}_-^A,\ \hat{Q}_5 = 2\hat{\sigma}_-^A \hat{\sigma}_-^B,\end{aligned} \tag{E2}$$

and f_j $(j = 1,2,3,4,5)$ are some time-dependent coefficients. Substituting Eq. (E1) into Eq. (11), we obtain a set of partial differential equations governing the coefficients of the $\hat{Q}$ operator,

$$\begin{aligned}
\frac{\partial}{\partial t} f_1(t,s) &= +2i\omega_A f_1 + \kappa_A F_1 f_1 + \kappa_B F_3 f_1 - iJ_{xy} f_3 - \kappa_B F_1 f_3 + \kappa_B F_4 f_3 + 2iJ_z f_4 + \kappa_A F_4 f_4 + \kappa_B F_3 f_4 - i\kappa_B F_5, \\
\frac{\partial}{\partial t} f_2(t,s) &= +2i\omega_B f_2 + \kappa_A F_4 f_2 + \kappa_B F_2 f_2 + 2iJ_z f_3 + \kappa_A F_4 f_3 + \kappa_B F_3 f_3 - iJ_{xy} f_4 - \kappa_A F_2 f_4 + \kappa_A F_3 f_4 - i\kappa_A F_5, \\
\frac{\partial}{\partial t} f_3(t,s) &= -iJ_{xy} f_1 - \kappa_A F_2 f_1 + \kappa_A F_3 f_1 + 2iJ_z f_2 + \kappa_A F_4 f_2 + \kappa_B F_3 f_2 + 2i\omega_B f_3 + \kappa_A F_4 f_3 + \kappa_B F_2 f_3 - i\kappa_A F_5, \\
\frac{\partial}{\partial t} f_4(t,s) &= +2iJ_z f_1 + \kappa_A F_4 f_1 + \kappa_B F_3 f_1 - iJ_{xy} f_2 - \kappa_B F_1 f_2 + \kappa_B F_4 f_2 + 2i\omega_A f_4 + \kappa_A F_1 f_4 + \kappa_B F_3 f_4 - i\kappa_B F_5, \\
\frac{\partial}{\partial t} f_5(t,s,s') &= +\kappa_A F_5 f_1 + \kappa_B F_5 f_2 - \kappa_B F_5 f_3 - \kappa_A F_5 f_4 + 2i\omega_A f_5 + 2i\omega_B f_5 + \kappa_A F_1 f_5 + \kappa_A F_4 f_5 + \kappa_B F_2 f_5 + \kappa_B F_3 f_5,
\end{aligned} \tag{E3}$$

where $F_j(t) = \int_0^t dsK(t,s)f_j(t,s)$ $(j = 1,2,3,4)$ and $F_5(t,s') = \int_0^t dsK(t,s)f_5(t,s,s')$, with the initial conditions:

$$\begin{aligned}
f_1(t,s=t) &= \kappa_A, \\
f_2(t,s=t) &= \kappa_B, \\
f_3(t,s=t) &= 0, \\
f_4(t,s=t) &= 0, \\
f_5(t,s=t,s') &= 0, \\
f_5(t,s,s'=t) &= i[\kappa_A f_2(t,s) + \kappa_B f_1(t,s)].
\end{aligned} \tag{E4}$$

Appendix F: Differential equations for coefficients of bosonic $\hat{O}$ in example 4

The coefficients in Eq. (85) satisfy the following differential equations

$$\frac{\partial}{\partial t} x_1(t,s) = i\omega_a x_1 + x_1 X_1 + x_2 X_1, \tag{F1}$$

$$\frac{\partial}{\partial t} x_2(t,s) = i\omega_b x_2 + x_1 X_2 + x_2 X_2, \tag{F2}$$

$$\begin{aligned}\frac{\partial}{\partial t} x_3(t,s) &= i\omega_b x_3 - x_4 X_2 + x_3 X_2 + x_2 X_3 \\ &+ x_3 X_3 - x_3 X_4 - x_2 X_4 - iX_5,\end{aligned} \tag{F3}$$

$$\begin{aligned}\frac{\partial}{\partial t} x_4(t,s) &= i\omega_a x_4 + x_4 X_1 + x_1 X_4 - x_1 X_3 \\ &- x_3 X_1 + x_4 X_3 - x_4 X_4 - iX_5,\end{aligned} \tag{F4}$$

$$\begin{aligned}\frac{\partial}{\partial t} x_5(t,s,s') &= i\omega_a x_5 + i\omega_b x_5 + x_5 X_1 + x_5 X_2 \\ &+ x_5 X_3 - x_5 X_4 + x_1 X_5 + x_2 X_5,\end{aligned} \tag{F5}$$

with the initial conditions

$$x_1(t,s=t) = 1, \tag{F6}$$
$$x_2(t,s=t) = 1, \tag{F7}$$
$$x_3(t,s=t) = 0, \tag{F8}$$
$$x_4(t,s=t) = 0, \tag{F9}$$
$$x_5(t,s=t,s') = 0, \tag{F10}$$
$$ix_5(t,s,s'=t) = 2(x_2 - x_1) + x_3 + x_4. \tag{F11}$$

and

$$X_j(t) = \int_0^t K(t,s)x_j(t,s)ds \ (j = 1 \text{ to } 4) \qquad \text{(F12)}$$

$$X_5(t,s') = \int_0^t K(t,s)x_5(t,s,s')ds \qquad \text{(F13)}$$

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